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Author(s):	Kippen, Karen Elizabeth Cruz, James Michael
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INSIDE

Mukund Mukundan

Driven to solve tough energy challenges

> "Our quality of life has always been intimately tied to our energy use throughout history."

Energy is a constant in Rangachary (Mukund) Mukundan's life—from his school years in India to today as a trailblazer in the Lab's applied energy program.

Having attended a high school where the motto was "knowledge is power," Mukundan took that axiom to heart. "Even today my passion is to increase my understanding of the world around us and to use that understanding to make a difference in people's lives," he said.

Although he began his college studies in metallurgical engineering, he quickly shifted to energy research, motivated by the environmental consequences. "Our quality of life has always been intimately tied to our energy use throughout history," he said.

At Los Alamos, Mukundan has focused on making the nation's transportation and electricity sectors cleaner and more efficient through understanding and controlling the electrochemical reactions at work in energy-producing technology.

In particular, he plays key roles in advancing the technology critical to transitioning to clean, renewable energy in both segments of the America economy.

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From Andrew's desk . . .

> Quantum science is advancing exponentially and is increasingly a subject of interest from funding agencies. This recent interest is due to quantum science's promise to make revolutionary advancements in, for example, computing, sensing, and communications. Advances in materials, new technologies, and novel algorithms will be needed to ultimately succeed within this field of research.

I would like to start off this message by adding my voice to other managers at LANL who are encouraging you all to get vaccinated against COVID-19. As you likely know, availability of the vaccine is no longer an issue. Anyone at LANL can email getvaccinated@lanl.gov to sign up to get vaccinated. If you have not already done so, I hope that you will start making a plan to get vaccinated today. Include your name, Z number, phone number where you can be reached, and your organization in the email. Remember, it's something you can do to help end the pandemic that has been such a disruptive force in our lives for over a year. In addition, if you have gotten your vaccine outside of LANL—for example, through the New Mexico Department of Health—please let Occupational Medicine know by sending a copy of your vaccination card to medical_records@lanl.gov.

On a more programmatic note, I recently led a committee of LANL staff members—including Malcolm Boshier (MPA-Q), Filip Ronning (IMS), Andrew Sornborger (CCS-3), and Sergei Tretiak (T-1)—to organize a LANL quantum science workshop that occurred in April. As you may know, and as discussed by MPA-Quantum Group Leader Leonardo Civale in his *MPA Materials Matter* note in this issue, quantum science is a strategic priority for MPA Division.

Quantum science is advancing exponentially and is increasingly a subject of interest from funding agencies. This recent interest is due to quantum science's promise to make revolutionary advancements in, for example, computing, sensing, and communications. Advances in materials, new technologies, and novel algorithms will be needed to ultimately succeed within this field of research. Progress will likely depend on integrated research with co-design efforts between many aspects of this field. For this workshop, we invited a diverse group of researchers from across LANL to speak about many of the current opportunities and challenges in the emerging area of quantum science. Our goals were to 1) educate the LANL community about some of the current challenges in various areas of quantum science, 2) learn about some of the ongoing quantum science at LANL, and 3) help initiate future collaborations among staff who may be interested in this rapidly emerging area. I believe that the workshop was very successful at meeting these goals. We had between 100–150 participants online throughout the workshop, which was kicked off by John Sarrao (DDSTE), Toni Taylor (ALDPS), and Irene Qualters (ALDSC). This representation is an indication of the broad interest in this area across LANL, and I am sure there will be more opportunity to engage in this space in the coming years as MPA Division, and LANL, establishes a leadership role in this emerging field.

MPA Division Leader Andrew Dattelbaum ■

From Leonardo's desk . . .

MPA-Q is the youngest group in MPA. It was created in November 2019, as a merging of MPA-CMMS and a portion of P-21, with a clear mandate to provide LANL with an internationally recognized group that can solve impactful interdisciplinary problems in quantum information science (QIS) and systems. I have been the MPA-Q group leader for about 11 months now, and navigating this "foundational period" surrounded by such an impressive group of people has turned out to be a great learning adventure: challenging at times; certainly never boring.

I sometimes reflect on how my own decisions along my career, combined with circumstances beyond my control, put me at this place today. Cuprate high temperature superconductors were discovered while I was a graduate student in Bariloche, Argentina. I abandoned my previous research and focused passionately on these new materials whose existence challenged decades of accepted knowledge, and I never stopped studying them. Following a strongly basic-science-oriented PhD thesis and as a postdoc at IBM (Yorktown Heights, NY), I developed an interest in applied research and technology. Back in Argentina, I continued my basic research in superconductivity while trying, unsuccessfully, to generate applied projects.

> "MPA-Q is now a group reaching maturity, and signs of progress and success are clear.

In 2002, I moved to LANL as the physics team leader of the Superconductivity Technology Center where, as the physicist surrounded by world-class materials scientists, I enjoyed one of the most successful and rewarding periods of my career. When the national superconductivity program ended and the STC was dissolved in 2012, Mike Hundley and my strongly correlated electron systems colleagues generously offered me a soft landing at CMMS. Fast forward, I was CMMS acting deputy group leader for several months in 2016 and 2019 and MPA acting deputy division leader during the first half of 2020.

I became the MPA-Q group leader in the middle of the pandemic. There were group members from the P-21 side whom I had never met personally, and in some cases, the work-from-home conditions precluded me from doing so for weeks. My learning curve has been steep, but I was aided by the support and commitment of our people. It took me a while to grasp the breadth of what we do at MPA-Q. We investigate materials to enable topological quantum computers and study exotic phases of quantum materials. We produce Bose-Einstein condensates at nanoKelvin temperatures to build atomic SQUIDs and gyroscopes. We support core LANL missions by exploring the properties of plutonium and the actinides. We use machine learning to design next-generation quantum technology. We make the most sensitive atomic magnetometers and use them to search for dark matter and explore the human brain. We study strongly correlated electron systems and unconventional superconductors. We develop quantum communication systems for a more secure electric grid. We stop and restart solid rockets. We design screening tools to protect the public from chemical warfare. We build remote-sensing instruments that land on Mars.

The appointment of Ray Newell as our deputy group leader completes our organization and marks the end of the beginning. MPA-Q is now a group reaching maturity, and signs of progress and success are clear. Funding is solid and diverse. We are already playing an important and growing role in QIS and the National Quantum Initiative, while maintaining, and even increasing, our strong portfolio of valuable non-QIS research and development. The interactions between the former two parts of the group grow by the day. We have a dense network of collaborations within MPA, across LANL, all over the US, and worldwide. I do not get lost in the basement of SM-40 anymore.

One year into the pandemic, there are clear signs that we will soon enter the post-COVID world. Nobody knows exactly what the "new normal" will be, but at MPA-Q we are all looking forward to it.

MPA-Q Group Leader Leonardo Civale ■

Mukundan cont.

Mukundan, a member of Materials Synthesis and Integrated Devices (MPA-11), said his hope is that his "research contributes a small part to these transitions that can lead to sustainable solutions to growing human energy demands."

Leading the charge

Mukundan is a deputy director for the Million Mile Fuel Cell Truck Consortium (M2FCT). This large-scale effort, co-led by Los Alamos and Lawrence Berkeley National Laboratory, aims to enable widespread commercialization of hydrogen fuel cells for zero-emissions heavy-duty applications.

He is also the LANL lead for the Hydrogen from Next Generation Electrolyzers for Water (H2NEW) consortium. H2NEW is co-led by the National Renewable Energy Laboratory and Idaho National Laboratory. This concerted effort focuses on overcoming technical barriers to enable affordable, reliable, and efficient electrolyzers, which have a key role in enabling the efficient and affordable production of hydrogen in a future clean energy economy.

Both consortia are funded by DOE's Hydrogen and Fuel Cell Technologies Office within the Energy Efficiency and Renewable Energy Office.

M2FCT and H2NEW are DOE's two high profile hydrogen related consortia, for hydrogen utilization and hydrogen production, said Program Manager Rod Borup (MPA-11). "Mukund's leadership and expertise are essential to the success of these consortia, which are designed to drive down costs by having the national labs, industry, and academia working together to significantly cut the cost and improve the performance of electrolyzers and heavy-duty fuel cells."

One of Mukundan's most challenging projects is aimed at developing non-aqueous flow batteries as energy storage devices. The project began as the concept of a few staff members just five years ago, Mukundan said, "when LANL had no significant presence in this area."

Funding from the Laboratory Directed Research and Development Program enabled the team to expand to include researchers with diverse backgrounds—and in turn establish itself as experts among the scientific community.

Now supported by the Office of Electricity, the project's ultimate goal is to develop flow batteries to where they replace the current generation of lithium-ion batteries for the purpose of large-scale energy storage in the nation's electric grid. Compared to lithium-ion batteries, flow batteries offer the prospect of improved durability and safety and longer lifetimes.

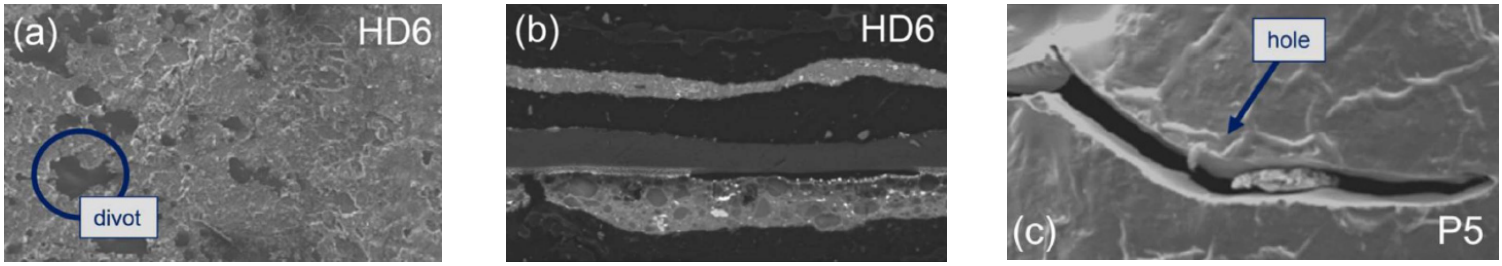
Finding the right environment

Mukundan is an Electrochemical Society Fellow, holds seven patents, and has authored more than 180 peer-reviewed journal and transaction papers.

After earning his PhD in materials science and engineering at the University of Pennsylvania, he joined the Lab as a postdoctoral researcher, impressed with the fuel cell and sensor research being done here. He became a staff member in 1999. Mukundan and his wife Harshini, acting group leader for Physical Chemistry and Applied Spectroscopy, have two children.

"Having lived in big cities all my life, I fell in love with the small town of Los Alamos that valued education and the sciences," he said. "I love the outdoors and like to hike, bike, and ski with my family and friends."

By Karen Kippen, ALDPS ■



Scanning electron microscope micrographs of membrane electrode assemblies after field operation, which demonstrate the (a) divot-type failure mode, in which (b) the catalyst layers pull away from the fuel cell proton exchange membrane (PEM) causing local thinning which leads to (c) local PEM tearing and failure. Reference: "Membrane accelerated stress test development for polymer electrolyte fuel cell durability validated using field and drive cycle testing," Rangachary Mukundan et al, *Journal of The Electrochemical Society,* 165 (6) F3085-F3093 (2018).

A new approach toward high-quality epitaxial actinide thin films

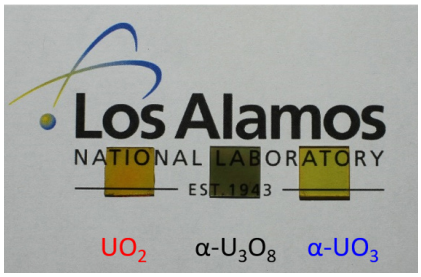
Technique benefits fundamental understanding and theoretical modeling of nuclear materials

For the first time ever, Los Alamos researchers—in collaboration with external researchers—have synthesized high-quality epitaxial UO_2, U_3O_8, and UO_3 thin films using pulsed laser deposition (PLD).

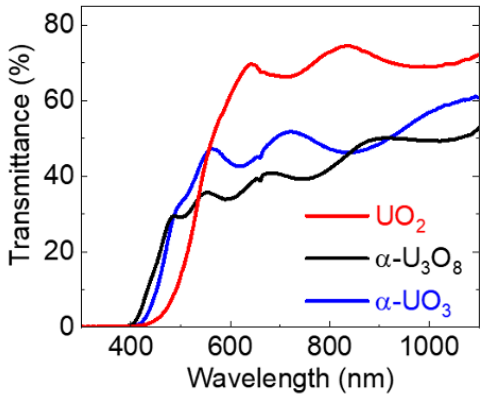
Uranium oxides have been considered as the most interesting actinide oxides because of their intriguing physical properties and technological significance in nuclear energy applications.

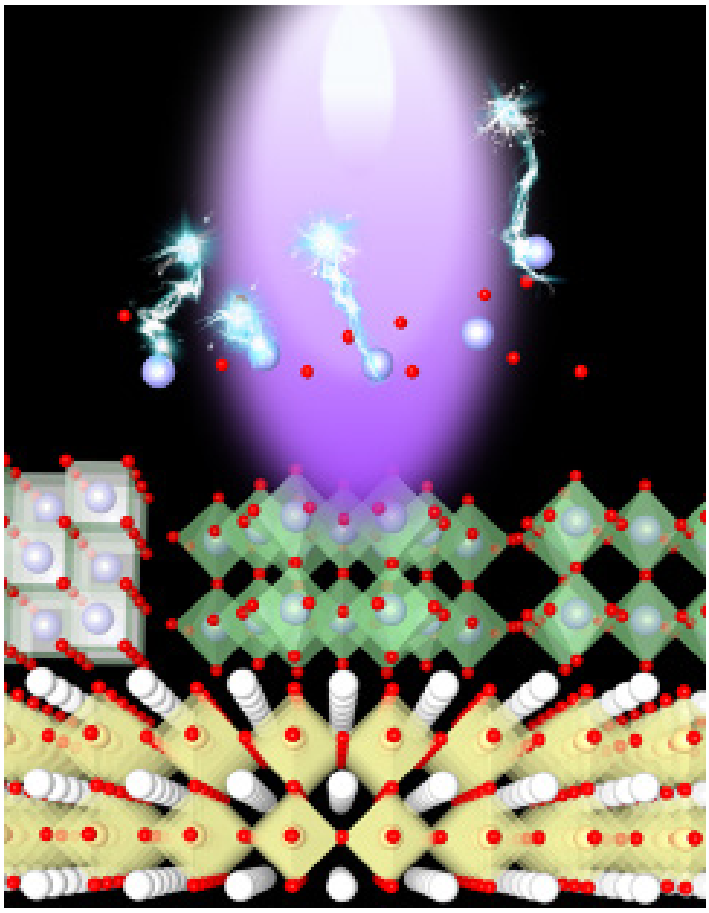
In particular, advancing the growth processes of uranium oxides will open new routes to develop novel correlated materials for future energy, sensing, and other applications. Given this technological significance and the rich physical and chemical properties of the UO_x material system, exploring the growth of high-quality epitaxial UO_x films with desired crystal structures and polymorphic phases is imperative.

In *ACS Applied Materials and Interfaces*, the researchers describe the successful use of PLD to grow three different types of UO_x thin films and explore the structural and optical properties. This production capability opens new avenues to explore applications and properties of a variety of actinide thin films.



Above: Photographs of epitaxial UO_2, α-U_3O_8 and α-UO_3 thin films grown by the PLD. Below: Transmittance spectrum for epitaxial UO_2, α-U_3O_8 and α-UO_3 thin films.





An illustration depicting formation of different phases of epitaxial UO_x thin films (middle region) by atoms in the plasma (purple oval) generated during the laser ablation on single crystal substrates (bottom).

In this work, the team systematically optimized the processing conditions for the epitaxial growth of the films with a high degree of control over both the phase and the structure.

The crystal structures and chemical valance states of the UO_x films were confirmed by Raman spectroscopy and x-ray photoelectron spectroscopy. The optical properties of these films are investigated by ultraviolet–visible spectroscopy. Additionally, the lattice vibrational modes of epitaxial UO_x films from Raman spectra were in good agreement with the density functional theory calculations.

The work leverages the Laboratory's capabilities and expertise in thin film growth and characterization and materials modeling and simulation.

The work, which supports the Lab's Energy Security mission and its Materials for the Future science pillar, was performed in part at the Center for Integrated Nanotechnologies, a

continued on next page ▶

A new approach cont.

DOE Office of Science Basic Energy Sciences user facility jointly operated by Sandia National Laboratories and Los Alamos National Laboratory. The Los Alamos portion of the work was funded by the Laboratory Directed Research and Development Program, with partial support from the Lab's G.T. Seaborg Institute.

Researchers: Aiping Chen, Erik Enriquez, Yogesh Sharma, Ibrahim Sarpkaya, Nicholas Winner, Paul Dowden, Han Htoon (Center for Integrated Nanotechnologies, MPA-CINT); Gaoxue Wang, Ping Yang, Enrique Batista (Physics and Chemistry of Materials, T-1); John Dunwoody, Joshua White, Andrew Nelson (Materials Science in Radiation and Dynamics Extremes, MST-8); and Hongwu Xu (Earth System Observations, EES-14).

Reference: "Structural and optical properties of phase-pure UO_2, α-U_3O_8, and α-UO_3 epitaxial thin films grown by pulsed laser deposition," *ACS Appl. Mater. Interfaces* 12, 35232–35241 (2020).

Technical contact:
Aiping Chen ■

MPA staff in the news

Lee receives NSERC postdoctoral fellowship

Chung Hyuk Lee (Materials Synthesis and Integrated Devices, MPA-11) has been awarded a Natural Sciences and Engineering Research Council of Canada (NSERC) Postdoctoral Fellowship. Lee's research focuses on designing and developing high performing fuel cell cathodes by tuning their porosity. He is planning to develop a novel platform that can precisely control the porosity and wettability of electrodes. His research aims to yield important insight into the transport properties of porous electrodes, guiding the next generation of electrode designs for electrochemical systems.

Lee, who earned his PhD in mechanical engineering from the University of Toronto, is a postdoctoral researcher on MPA-11's Fuel Cells and Electrochemical Sensors Team. He is mentored by Rangachary Mukundan and Jacob Spendelow (both MPA-11).

NSERC is a federal research funding agency mandated to promote and support postsecondary-based research and training in the natural sciences and engineering. Fellowship recipients are selected based on their research ability and potential and communication, interpersonal, and leadership abilities. ■

Winter elected member-at-large of APS GIMS

Laurel Winter (National High Magnetic Field Laboratory-Pulsed Field Facility, MPA-MAGLAB) was elected member-at-large of the American Physical Society (APS) Topical Group on Instrument and Measurement Science (GIMS). The topical group was formed in 1984 and aims to provide professional recognition to those who advance instrument and measurement science in all fields of physics. As a member of its executive committee, she will support its mission to advance the development of new instrumentation and measurement science and to provide a forum for discussion of these topics. Her three-year-term runs through March 2024, during which she will serve primarily as a liaison between the membership and the executive committee.

Winter is the Pulsed Field Facility's user program director. At the LANL magnet lab, she focuses on condensed matter physics at low temperatures and high magnetic fields with an emphasis on strongly correlated electron systems and heavy fermions. She received a BA in physics from Clark University in 2009 and a PhD in physics from Florida State University in 2015. ■

Jaime named AAAS Fellow

Marcelo Jaime (National High Magnetic Field Lab-Pulsed Field Facility, MPA-MAG) has been named a fellow of the American Association for the Advancement of Science (AAAS). He was cited for "distinguished contributions to the field of experimental physics, particularly for the study of strongly correlated electron systems and quantum phase transitions in extreme magnetic fields." Election as AAAS Fellow is an honor bestowed upon AAAS members by their peers. Members have been awarded this honor by AAAS because of their scientifically or socially distinguished efforts to advance science or its applications.

At the mag lab, Jaime, who has a PhD in physics from the Instituto Balseiro, Bariloche, Argentina, has developed techniques to measure thermal properties in very high magnetic fields, pulsed and continuous, at low temperatures. ■

HeadsUP!

7 ways to avoid a hungry bear at the dumpster

With a gradual increase in the on-site workforce, conditions are ripening for bear encounters. Human food is calorie-rich and can be easy for bears to get. To help keep bears away, bear-proof dumpsters have been deployed across the Laboratory at areas with a history of bear and trash issues. When used properly, a bear-proof dumpster can keep human trash in—and bears out.

How do you know a dumpster is bear-proof?

- It's brown with a number placard that starts with a “B”
- It has a "Be Bear Aware" sticker on it
- There are smaller doors on the dumpster lid
- You can see carabineer clips and bars

When properly secured, the smaller doors on the dumpster lid are shut and the carabineer clips and bars properly attached.

7 ways to reduce running into hungry bears

Take the following steps when approaching a dumpster:

- Look to see if the dumpster is properly secured (lid closed, carabineer latched, and bar in place);
- If approaching a dumpster in a vehicle, honk your horn, it may scare a bear out of an unsecured dumpster;
- Look for trash outside or liquid dripping down the side of the dumpster;
- Look for scratches and paw prints on the side of the dumpster;
- Listen for sounds and rustling inside the dumpster;
- If you see a bear in or near a dumpster, stop and step away; and
- When you're in a safe location call the EOC (667-2400).

What if you encounter an aggressive bear or predator?

First things first: Stay calm. Next:

- Talk in a low voice to reassure the bear or other large wildlife that you aren't a threat, and back away slowly to the safety of a building or vehicle,
- Don't run; running triggers the animal's instinct to chase,
- Watch for younger animals; a mother mountain lion or bear may move to protect cubs,
- If a bear or other large animal approaches you and/or becomes aggressive, arm yourself with a large stick, throw rocks or sticks at it, and speak louder in a firm voice, raise your arms to look larger,
- If attacked by a bear or other large wildlife, fight back using any objects available, such as rocks, sticks, backpacks, jackets, hands, and feet. When safe to do so call the Emergency Operations Center at 7-2400, or if in need of medical attention, call 9-1-1.

Celebrating service

Congratulations to the following MPA Division employees who recently celebrated a service anniversary:

Christopher Leibman, MPA-11 . . . . . 35 years
Anatoly Efimov, MPA-CINT . . . . . 20 years
Jon Baldwin, MPA-CINT . . . . . 15 years
Julie Montoya, MPA-11. . . . . 15 years
Sandipkumar Maurya, MPA-11. . . . . 5 years
Stefan Williams, MPA-11 . . . . . 5 years

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To submit news items or for more information, contact Karen Kippen, ALDPS Communications, at 505-606-1822 or aldps-comm@lanl.gov.

To read past issues see www.lanl.gov/orgs/mpa/materialsmatter.shtml.